Modeling Biological Systems

Principles and Applications

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statement of what the model is intended to do. Other disciplines may not require for publication such a self-conscious and direct statement, but, at some point, the modelers probably do.

5 Exercises

1. To what extent has Innis incorporated Overton's criteria for objectives statements?
2. How good was the objective statement of the "doubling time" model?
3. Using Innis' statement and Overton's criteria as guides, write an objective statement for the following problem: "How many cases of AIDS will occur in Utah in 1999?" Would the objectives change if the location had been San Francisco? Why or why not? What role does spatial scale of extrapolation play in this problem?
4. Write an objective statement for the leaky bucket problem of Chapter 1.
5. Write an objective statement for this problem: "What should be the best grazing pressure on the Foobar National Forest to simultaneously maximize cattle production and forest quality?"
6. We noted in the discussion of the model of the world's population that our abilities to validate the model were limited by our inability to replicate the system. Under what circumstances, if any, is it worth while to model systems that cannot be replicated or tested using rigorous statistical methods?
7. Read pages 10–13 in Reckhow and Chapra (1983b) and decide if there is a need to distinguish *validation* and *corroboration*.
8. Read an article in a current journal describing a model and critique the objective statement. In the models described in the chosen journal, how many discuss validation?

Chapter 3

Qualitative Model Formulation

3.1 How to Eat an Elephant

BUILDING a model is like eating an elephant: it's hard to know where to begin. As with almost all problems, it is helpful to break a big problem into smaller, more manageable pieces. We do this with model formulation (Fig. 2.1) by first creating a *qualitative* model and then converting this to a *quantitative* model (Chapter 4). Qualitative model formulation, then, is the conversion of an objective statement and a set of hypotheses and assumptions into an informal, conceptual model. This form does not contain explicit equations, but its purpose is to provide enough detail and structure so that a consistent set of equations can be written. The qualitative model does not uniquely determine the equations, but does indicate the minimal mathematical components needed. The purpose of a qualitative model is to provide a conceptual framework for the attainment of the objectives. The framework summarizes the modeler's current thinking concerning the number and identity of necessary system components (objects) and the relationships among them.

Qualitative model formulation is not always explicitly performed. If a modeling project is simple enough, elaborate plans for writing the equations are not necessary. Most of us do not need detailed instructions for getting out of bed in the morning. But with large models having many variables that interact in complicated ways among themselves and with the environment, it is easy to become confused. By providing an overview of the system, a qualitative version of the model can help reduce this confusion.

Qualitative models can take any form (except mathematical), but diagrams are the usual representation. Given our emphasis on differential equations and compartment models, three important diagrammatic schemes are: *block structure* diagrams (having origins in electrical engineering and analog computers), *Odum energy flow* diagrams (similar to block structure diagrams but based on energy flow within ecosystems), and *Forrester* diagrams (having origins in systems analysis and operations research). All

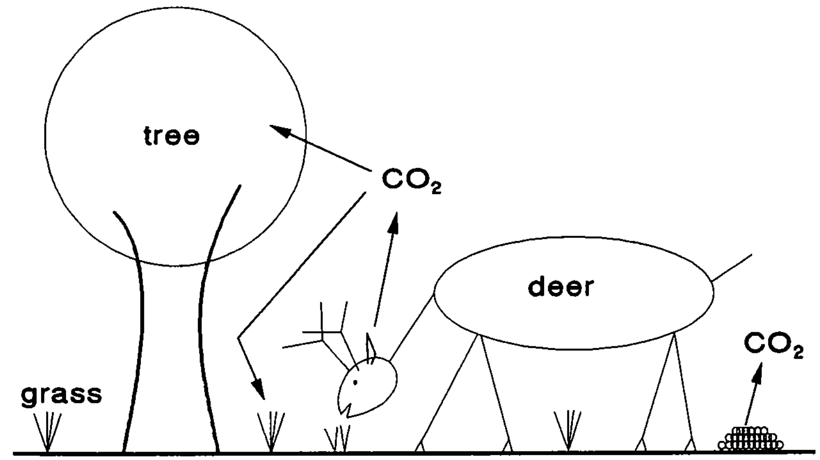

Figure 3.1: A simple ecosystem in which carbon moves among the labeled components.

three share the ability to represent systems as a set of objects and their interrelations. We will stress the latter here, but the interested reader can learn more of block structure diagrams in (Shannon 1975) and Odum energy diagrams in (Odum 1971).

3.2 Forrester Diagrams

Forrester diagrams (Forrester 1961) were invented by Jay Forrester, an MIT professor famous for work on early digital computer hardware and the simulation of social systems. Forrester diagrams are designed to represent any dynamic system in which a measurable quantity flows between system components.

Consider a simple ecosystem in which carbon flows between a population of grass and a population of deer (Fig. 3.1). Let us suppose that our objectives suggest that only deer and grass are interesting and that the grams of carbon in these two components are the relevant measures. Because of our simplification, we will not explicitly consider other components that may have large quantities of C (e.g., atmospheric CO_2 and excretion by deer). Consequently, two numbers (grams of carbon in grass and grams of carbon in deer) completely specify the condition of the system at a moment in time. By accepting this simple view of the ecosystem, we are stating that other variables or quantities are irrelevant and do not add to our knowledge of the system. For example, other consumers (e.g., insects), producers (e.g., the tree), or other variables (e.g., nitrogen) are not important. Moreover, these two numbers may change in time so that the condition of the system is dynamic. The exact nature of the temporal changes depends on the rates of flow of carbon into the grass component (growth) and into the deer population (grass consumption).

Figure 3.1 is a crude qualitative model in diagram form of the system, but since it makes specific reference to *deer* and *grass*, it has limited application to other systems. We want an abstraction of the basic concepts of *system components* and *material flows* to obtain a general tool for qualitative modeling of systems. Forrester diagrams are such an abstraction.

To understand the basis of the diagramming scheme, recall the general definition of a system: *a collection of objects and relations among them.* There are two kinds of objects: (1) those that are inside the system and are explicitly modeled and (2) those that are outside the system and are not modeled. The internal objects are called *state variables* and are those that, taken all together, characterize the condition or *state* of the system. In the example above, the state variables are *grass* and *deer.* These variables are dynamic and change their state over time. (See Caswell et al. 1972 for a more rigorous definition of state variable.)

The outside or external variables are either sources or sinks and are not modeled explicitly (i.e., no equations are written for these). For example, atmospheric CO_2 is both a source and a sink. It is a source because it represents an unmodeled pool of C that is an input to a state variable (grass). It is also a sink since gaseous CO_2 is a product of deer respiration.

Each state variable is described by its current level of the quantity of interest: the quantity in which units we measure the state of the variable (e.g., numbers of individuals, grams of carbon, temperature, etc). *Relations* between system objects have two forms: (1) the direction and rates of flow between the quantity of interest and the objects and (2) the influences of a variable (e.g., the quantity of interest) on the rates of flow.

Forrester diagrams are direct graphical representations of these concepts that permit easy translation to mathematical equations. They can be thought of as a graphical "language" with phrases that can be connected in certain prescribed ways. The graphical vocabulary items of the language are listed in Fig. 3.2 and are described below.

Objects System objects are the state variables of the system (called *levels* by Forrester). They are the primary system components whose values over time we wish to predict. They are dynamic quantities and are represented by a rectangular box (Fig. 3.2a). The box should contain a mnemonic name for the object and its unit of measurement. Many descriptions of models of this type refer to levels as *compartments*, and the type of models being represented by Forrester diagrams as *compartment models.*

Material Flows Flows are one manifestation of relations between system objects, which we will call a *flow relation.* A flow is represented as a solid arrow (Fig. 3.2b) and identifies the pathway over which the quantity of interest (e.g., grams of carbon) flows. In most models, the rate of flow is a dynamic quantity that is influenced by system components, and this rate is symbolized by a *control valve* (the "bow-tie") on the flow relation.

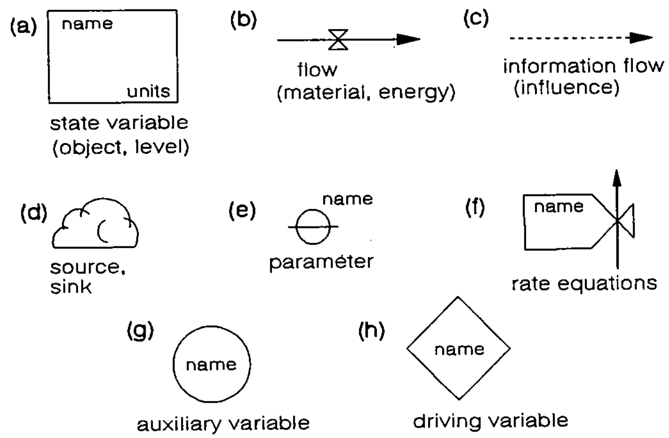

Figure 3.2: The basic components of a Forrester diagram.

Information Flow or Influences The second manifestation of relations between objects are the effects that the quantity of one object has on the rates of inputs to or outputs from another object (e.g., effects on growth rates). These are *control relations.* State variables affect the control valves of material flows of other state variables (including themselves). These influences are represented as *information transfers* (dotted arrows in Fig. 3.2c) connecting state variables and control valves. The tail of the arrow indicates the influencing component and the head of the arrow indicates the affected rate. Possible sources of information transfer are state variables, parameters, driving variables, and auxiliary variables or equations.

Sources and Sinks Objects that are defined to be outside the system of interest, but which are inputs to state variables or outputs from state variables, are represented as "clouds" (Fig. 3.2d). They are not state variables since they are not modeled explicitly and are not represented by dynamic equations. (Hence, they are nebulous and vague — traits well represented by clouds.) Sources or sinks cannot be involved in an information transfer. That is, they cannot alter a rate, nor can their condition be altered.

Parameters Constants in equations are noted in the diagrams by small circles with lines (Fig. 3.2e). They invariably are used as the tail of an information transfer, since their values influence flow rates and other equations within the model. Since they are constants, their values are not changed by an information transfer.

Rate Equations Total (or absolute) rates of input to, or output from, a state variable are described mathematically with *rate equations.* It is useful to identify and label these explicitly by modifying the control valve symbol (Fig. 3.2f). The equations usually describe information transfers from state variables and parameters.

Auxiliary Variables and Equations Auxiliary *variables* (large circles, Fig. 3.2g) are variables that are computed from an auxiliary *equation.* The auxiliary equation can be a function of other auxiliary variables, state variables, driving variables, and parameters. Auxiliary variables change over time because they depend on either (a) a state variable, (b) a driving variable that depends on time, or (c) an auxiliary variable that depends on a state variable or driving variable. Auxiliary variables are never constants, nor are they state variables.

Auxiliary variables are primarily used to simplify the writing of rate equations. In this use, they may be substituted into the equation, but they are isolated for clarity or computing efficiency (they may be used by several state variables). Consequently, they are often shown influencing rate equations. A secondary use is to convert, for output purposes, a state variable or another auxiliary variable.

Driving Variables Dynamic events that relate to variables that are not state variables (e.g., season or temperature in some models) are often used as *forcing functions.* These driving variables are represented as large diamonds (Fig. 3.2h). Driving variables may take as input only other driving variables. Usually, they have no inputs and time is assumed to be a component of the variable (e.g., temperature values on different days). Here are two examples when one driving variable may influence another: (1) A driving variable of time could influence a driving variable that specifies temperature over space. The temperature at depth (space) in a water column could be influenced by season (time): different temperatures at depth at different seasons. (2) A driving variable of time at one scale (slow) could be used to determine a variable that occurs at a faster time scale [e.g., season (a slow time-dependent driving variable)] can influence hourly temperature values (a fast time-dependent driving variable). The units of the driving variable (e.g., time, space) should be specified in the diagram.

3.3 Examples

As illustrations of this diagramming technique, we consider some simple examples.

3.3.1 Grass–Deer "Ecosystem"

Consider a system composed of grass and some deer that eat the grass (Fig. 3.1). For the sake of definiteness, we will make the following biological assumptions.

1. The per capita rate of growth of grass (g C produced per g C of existing grass) is constant. Therefore, the total growth will be the per capita rate times the total amount of C present.
2. The only loss to the quantity of C in the grass population is by deer consumption.

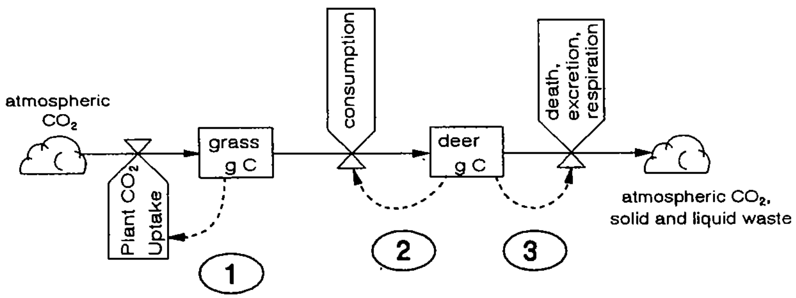

Figure 3.3: Forrester diagram for the grass–deer ecosystem. Solid arrows are pathways for C flow; dotted arrows represent relations between levels and input or output rates as hypothesized. (Numbered ellipses on information flows are not part of Forrester diagrams, but are used for explanatory purposes only.)

3. Deer compete with one another for grass so that, as the quantity of deer increases, each deer receives less C.
4. Deer excrete or respire a fixed proportion of their existing C as either atmospheric C or solid/liquid waste.

None of these hypotheses are detailed enough to allow us to uniquely define the equations, but they do permit us to draw the Forrester diagram in Fig. 3.3.

The assumptions indicated only two state variables: grass and deer. Therefore, there are only two boxes (levels) in the Forrester diagram. Also from our assumptions, there are only three flow relations: source to grass, grass to deer, and deer to sink. The diagram implies that any other flows are assumed to be unimportant to the objectives of the model. For example, we explicitly precluded C from flowing directly from grass back to the atmosphere or another sink. Information transfer 1 is a diagram of the concept that total grass growth depends on the amount of grass present. Information transfer 2 is similar, but we know from our verbal statement that deer are competing with one another, and grass is not competing (per capita rates are constant). Therefore, given the similarity of information transfers 1 and 2 (Fig. 3.3), it is clear that different hypothesized control relations can have the same Forrester diagram presentation. This implies that a single Forrester diagram can represent many different sets of hypotheses. Forrester diagrams do not uniquely determine the model equations. Information transfer 3 represents the effect of deer on the loss rate of C from the deer population. The verbal statement of this control relation is similar to that for grass growth rate, so the information transfer arrow is similar.

3.3.2 Population Growth with Explicit Birth and Death

To demonstrate the relation between diagrams and equations, the next example will start with an equation and produce a consistent diagram.

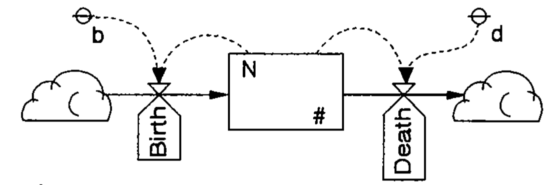

Figure 3.4: Forrester diagram for one form of the density-independent population growth model.

The classic, density-independent population model written as a finite difference equation (FDE) is $N_{t+1} = N_t + rN_t$, where r is the net per capita growth rate. Suppose we reparameterize it using the identity $r = b - d$, where b is the per capita birth rate, d is the per capita death rate, and both are positive quantities:

$$N_{t+1} = N_t + bN_t - dN_t. \tag{3.1}$$

Note first that there is a single state variable (N); therefore there will be a single box in the Forrester diagram. In general, there will be exactly as many boxes (levels) and FDEs as there are state variables. Second, note that Eq. 3.1 has two components of change: a positive value (bN_t) and a negative value ($-dN_t$). These correspond in Forrester diagrams as inputs to and outputs from a single state variable. Thus, for this form of the model, we have a Forrester diagram as shown in Fig. 3.4. Note the use of clouds (sinks and sources) to represent the origin of newborn individuals and the destination of dead individuals.

To illustrate the use of auxiliary variables and equations, consider the case where birth rates decrease linearly as numbers of individuals increase, but total death is a simple proportion of the population:

$$N_{t+1} = N_t + bN_t \underbrace{\left(1 - \frac{N_t}{K}\right)}_{R} - dN_t. \tag{3.2}$$

The second (middle) term of the right-hand side is the absolute rate of births in the population. The third term is the absolute rate of death. Birth rate is determined by a "reduction factor" that approaches zero as N approaches a constant K [i.e., $(1 - N/K) \to 0$ as $N \to K$]. Our modeling objectives might suggest that this is a particularly important quantity (e.g., we want to examine a range of functional forms, not just the linear one above). Consequently, we isolate that subexpression with a special symbol (R) and we treat it as an auxiliary variable. Figure 3.5 shows the Forrester diagram for this model. Note that it is similar in form to Fig. 3.4, but that we have used an auxiliary variable to represent the effect of density on the reduction factor. The "effective" per capita birth rate is bR, where b is the maximum per capita birth rate. Note that R is a function of N (state variable) and K (a parameter), so information transfer arrows

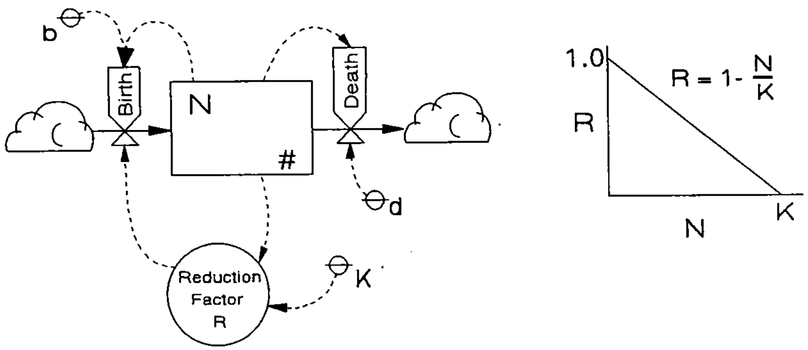

Figure 3.5: Forrester diagram for one form of density-dependent population growth model.

connect these entities with R.

It is somewhat a matter of taste to separate R and b. Alternatively, we could draw the diagram using a different auxiliary variable, perhaps called "effective per capita birth rate," corresponding to the variable $b(1 - N/K)$. This would require a minor modification of the control relations (information transfer arrows). Finally, it is possible to draw the Forrester diagram for Eq. 3.2 without any auxiliary variables; it depends on the emphases the diagrammer wishes to achieve.

3.3.3 Net Population Growth

The above models used explicit birth and death to show the relations between the parameters governing increases and decreases, and the input and output arrows in the diagrams. The typical presentation of these models subsumes birth and death into a net rate parameter r, which may be positive or negative. For these forms, the corresponding diagrams for the two models (Fig. 3.4 and Fig. 3.5) are shown in Fig. 3.6. Note the double-headed material flow arrows used to indicate that the parameter r controls both the inflow (away from source) as well as outflow (toward the sink). The single cloud serves a double purpose here as both sink and source.

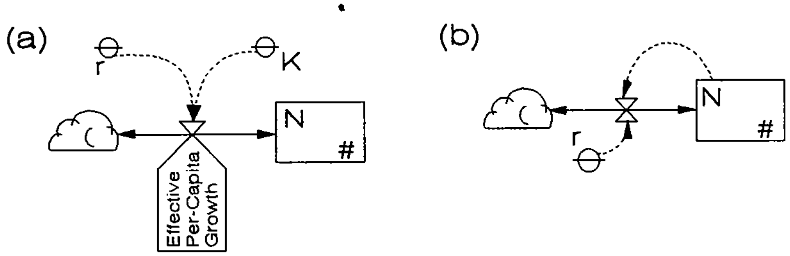

Figure 3.6: Forrester diagrams for density-dependent (a) and density-independent (b) growth using the normal parameterization.

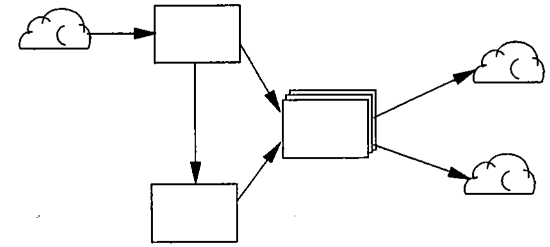

Figure 3.7: Forrester diagram showing multiple state variables. The set of three offset boxes represents three state variables all of which have the same relations (inputs and outputs) to other state variables in the system.

3.3.4 Multiple State Variables

It is often clearer to isolate different inputs and outputs to a state variable, even though they may be additive and could be lumped. This may be important if the controls on the different rates vary significantly, usually due to different parameters. This is diagrammed by multiple material flows into or out of a level.

When a model has more than one state variable (e.g., an ecosystem model with equations for plants, herbivores, and carnivores), then each object is represented by a box (level) that connects with the others according to the flow of material (energy) defined by the relations (i.e., foraging relationships). Figure 3.7 illustrates this for a simple case. The critical point for models of this type is that the units of state variables and the units of flow must agree. Some models have state variables that possess identical inputs and outputs (e.g., discrete soil layers in a water flow model); to simplify the diagram, these are shown as offset boxes (Fig. 3.7). A similar scheme can be used for auxiliary variables.

A more complicated case is illustrated in Fig. 3.8 for a simple agroecosystem model in which there are fertilization regimes, pests, and crop harvesting schedules. In this model, suppose the broad objective is to *determine the effects on profits of different schedules of fertilizer and pesticide applications to fields of alfalfa.* By "schedule," we mean the timing and amounts of applications. The major pests of alfalfa are weevils and aphids, but these are dynamic since pesticides will kill some of them. So, at least one state variable must represent the pests. We are also interested in the effects of fertilizer applications, but this also will be dynamic (it is applied at certain times and in variable amounts). Consequently, another state variable should be the soil nutrient pool. As we are primarily interested in the profits of farmers, we will need to know both the amounts of crops in the field and the amounts harvested.

Thus, the state variables are: nutrients, insect pests, field alfalfa, and harvested alfalfa. All of these must have common units, so for the sake of the example, we will assume that nitrogen is the limiting nutrient to be added and that all other state variables will be quantified in units of

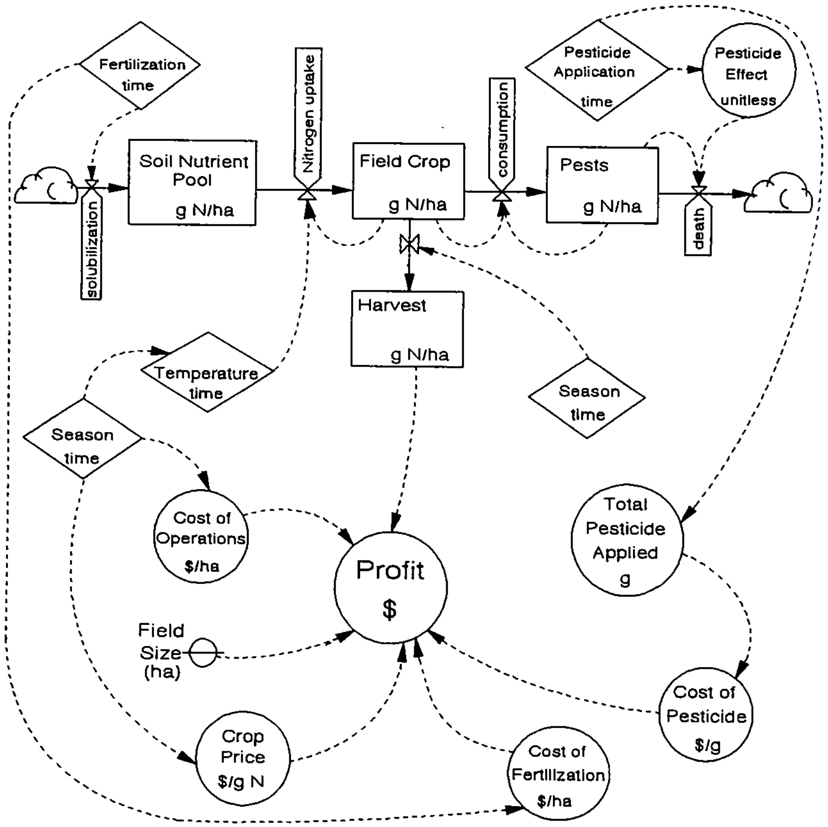

Figure 3.8: Forrester diagram for a hypothetical agroecosystem model showing multiple state variables of an agricultural system.

g N/hectare. These are not the most natural units by which to measure alfalfa and insect pests, but we can always use a conversion factor (auxiliary variable) to create other units.

The scheduling of management events such as pesticide application and fertilization is represented by driving variables, as are natural events such as season and temperature (Fig. 3.8). The objectives state that one of our primary interests is farmer **Profit**. Because we have chosen the dynamics to be stated in units of g N/ha and the units of profit are dollars, we need to convert from g N/ha harvested to dollars. To accomplish this, we use auxiliary variables such as **Fertilization Cost** ($/ha), **Field Size** (ha), **Alfalfa Price** ($/g N), and so on (Fig. 3.8).

The diagram is not complete because we have omitted the parameters, but without more specific hypotheses on the dynamics of the components it is difficult and not useful to add this facet of Forrester diagrams. The reader should study Fig. 3.8 so that the components (levels) and flows (material and information) are clear. In particular, it should be evident how a mathematical model based on this diagram will address the original objectives.

3.3.5 Multiple Flow Variables and Units

When different units on flow variables are modeled (e.g., g N and g C or blood pressure and blood oxygen in a physiological model), *parallel* models (or *multiple models*, Rideout 1991) must be used to avoid having "apples" flow into "oranges." The dynamics of many biological processes depend on several interacting variables. There are two broad applications of this concept in modeling: (1) the variables are at the same level of biological organization but may interact in their influence on the dynamics, or (2) the variables are at different levels of organization, but both are needed to address the model objectives.

Two variables (A and B) are on the same level of biological organization if all of the measurements that can logically be made on A can also be made on B, *and* there are no measurements that can be made on B that cannot be made on A. So, for example, two chemical molecules (CO_2 and H_2O) are on the same level because we can measure on both such things as molarity, boiling point, molecular weight, and so on. In contrast, an individual organism and a population of organisms are on different levels of organization since we can measure population growth rate on the population, but not on a single organism.

Variables that are on the same level of organization may interact to affect some biological process negatively (negative feedback), positively (synergism), or independently (substitutable). For example, the electrical potential across the membrane of a nerve cell is determined by the difference between the net charge inside the cell and the net charge outside the cell. Therefore, two variables that might be modeled and that interact negatively are positive ions exemplified by potassium (K^+) and negative ions such as chloride (Cl^-), since the net charge is the sum of positive and negative ions. In other situations, two different variables might complement each other and enhance the rates of change of biological processes [e.g., nerve cell activity and electrical potential and the different forms of positive ions: K^+ and sodium (Na^+)]. In still other systems, the two variables may influence dynamics independently, for example, grass species A and B may each increase deer growth rates by an equal amount.

In all of the above examples, it is conceivable (but not necessary) that a model would portray the dynamics of both quantities (K^+ and Na^+, or species A and B). In all three possibilities, if we wish to describe the dynamics of the affected process as influenced by the variables, then we must describe the dynamics of the individual variables and their effect on the process. Therefore, since the physical quantities cannot flow among themselves (i.e., g K cannot flow from a compartment containing g Na), we represent the separate dynamics as parallel models.

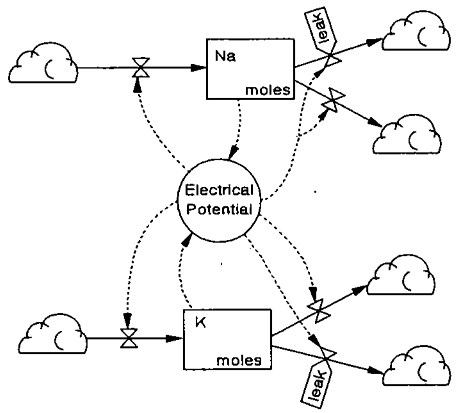

Figure 3.9: Forrester diagram when multiple flow variables are used. Unlabeled material transfers are assumed to be losses or gains caused by ion pumping.

An example of variables at different levels of organization is variables describing the size of individuals and population size. In models in which the growth rate of the population is influenced not only by the current numbers of individuals in the population, but also by the average body size (e.g., through the feeding rate), both quantities must be modeled. Obviously, these are two very different kinds of quantities and it is absurd to suppose that they can be related by a material transfer (solid arrow in a Forrester diagram). It makes no sense to say that average body size "flows" into numbers of individuals. Consequently, in a model, these two variables must be kept separate.

To illustrate this concept graphically, consider a very simple model of nerve cell activity. The activity level is measured as the electrical potential across the nerve cell membrane. This is determined by the relative concentration of K^+ and Na^+ on the inside. Ions of K and Na flow into the cell through ion-specific channels at rates that depend on the current electrical potential of the cell. Figure 3.9 shows one implementation of the integration of the dynamics of K and Na to determine electrical potential. Since K and Na are different quantities, they are not interchangeable and therefore must have different inputs, outputs, and level representation.

Care must be exercised when diagramming to recognize differences in units between state variables. Units that are superficially the same can in some circumstances be completely different. Often these differences are hidden by the mathematical equations. For example, if our interest is in the flow of carbon between components of a plant (e.g., leaves and roots) in a plant growth model, then an atom of carbon in the leaves can actually become incorporated into the roots. In contrast, suppose our interest is in a model of the population dynamics of a species of plant and its herbivore and the "flow" variable of interest is numbers of individuals in each population. It does not make sense to say that individual plants flow into individual

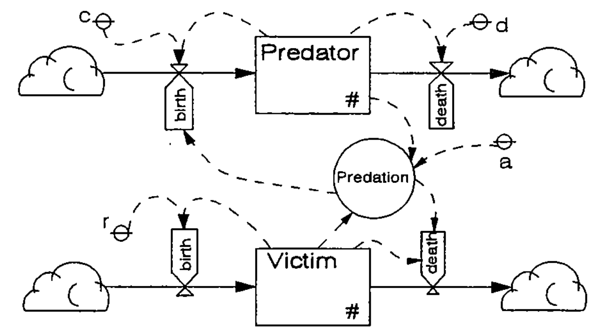

Figure 3.10: Simplified Forrester diagram for linked population models based on numbers of individuals.

consumers. The biomass of the plant in fact does become incorporated into the biomass of individual herbivores, but the numbers in the population are created by processes of birth and death. The basic concept here is one of "conserved" and "nonconserved" flow quantities. Grams of carbon is a conserved quantity; it is the mass of a physical object. And, except under unusual physical circumstances, an atom of carbon is never created or destroyed. Numbers of individuals are not conserved in the same way. Prior to birth the individual did not exist, although all of its atoms were present in other forms. At its death, the individual is destroyed, but its constituent atoms persist.

This distinction influences the way Forrester diagrams are drawn for some types of models. In predator–prey models, when numbers of individuals are modeled, the units are actually numbers of prey individuals and numbers of predator individuals. These units are as incompatible with each other as were the units in Fig. 3.9 and the diagram should use parallel models. Consequently, we should use a Forrester diagram similar to the simplified form shown in Fig. 3.10.

3.4 Errors in Forrester Diagrams

Below is a short list of some of the errors that can be made in drawing Forrester diagrams (see Fig. 3.11).

1. Using any symbols other than those defined in Fig. 3.2. For example, there is no symbol like a solid line with no arrowhead attached (Fig. 3.11a).
2. Failing to label all boxes, variables (auxiliary and driving), and parameters with names and units (where appropriate, Fig. 3.11a).
3. Showing sources or sinks influencing rates (Fig. 3.11b).
4. Showing rates influencing state variables (Fig. 3.11c).
5. Showing material flows (solid arrows) between objects other than state variables and sources and sinks (Fig. 3.11d).

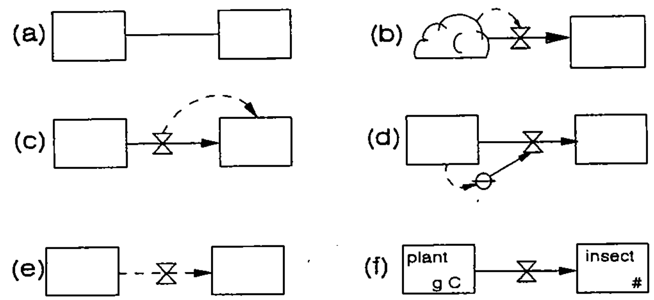

Figure 3.11: Examples of incorrect Forrester diagram fragments.

6. Showing an influence on a quantity that cannot change (e.g., a parameter, Fig. 3.11d).
7. Showing information flows between state variables (Fig. 3.11e).
8. Using incompatible units of flows or state variables (Fig. 3.11f).
9. Using state variables that are not in the model (objectives or equations) or not including state variables that are in the model.

3.5 Advantages and Disadvantages of Forrester Diagrams

Many modelers and theoreticians do not use Forrester diagrams and believe they only get in the way. There is an important element of truth in this view. The equations are the primary objects of interest. Their solutions, not the diagram, produce the output used to address the model objectives. Moreover, the diagrams are not always a compact representation of the model. As the number of state variables, parameters, and relations between objects become large, the size of the diagram increases. Complex diagrams can span several pages, in which case much of the heuristic value is lost.

There are, however, three situations in which Forrester diagrams are useful. First, in learning the rudiments of the modeling process, it is helpful to separate the trauma of mathematical equations from the conceptual issues of the nature of system objects, the characteristics of the material flows between them, and the controls on the dynamics by internal influences. A graphical language has this potential.

Second, many people who are not mathematicians and to whom a model must be explained react favorably to the graphical representation. For most variables and flows, there is a natural correspondence between a material flow and a physical or biological process (e.g., consumption in a foodweb), or between a state variable (boxes) and a compartment (e.g., population). These are concepts with which most people have some experience. As a consequence, understanding is more quickly attained, and constructive criticism (or, even, agreement) is more readily achieved. Moreover, although mathematics offers opportunities for an extremely compact representation

of complex relationships, models attempting to achieve a high degree of precision or realism will often require complicated equations. The mathematical expressions for driving variables are often an example of this since they can represent seasonal effects on physical variables such as temperature. Forrester diagrams can reduce some of this complexity by subsuming the mathematical details in a simple symbol.

Finally, Forrester diagrams can be a valuable aid in organizing the computer simulation program. Each level effectively becomes a program module; the set of input and output arrows are components that increase and decrease the finite difference equations. The parameters are the data on which program module operates. Input information flows and parameters indicate arguments to the subroutine; output information flows indicate subroutine side effects (changed variables).

Clearly, there is a point at which diagram complexity obfuscates the basic structure of the model and frustrates attempts to effectively communicate. Just as we must provide objectives for models, we must also recognize our objectives in presenting a model in one form or another. The choice will depend on whether we are communicating with politicians, managers, mathematicians, computers, or our biologist colleagues.

3.6 Principles of Qualitative Formulation

The first rule of discovery is to have brains and good luck. The second rule of discovery is to sit tight and wait for a bright idea.

— Polya (1973)

Qualitative model formulation is one of the sub-problems in the modeling activity. We wish to discover the simplest description of a system that will satisfy the objectives. This section describes a few basic principles that apply to all attempts to formulate a qualitative compartment model using Forrester diagrams. Many of the principles will also apply to other modeling approaches. Based on the Forrester diagrams shown thus far, it should be clear that the purpose of the principles is to help you

- Identify the state variables (levels)
- Identify the flows among the state variables
- Identify the controls on the flow rates
- Identify the auxiliary and driving variables.

To accomplish the above, answer the following questions.

1. *What are the questions to be answered?* Write down all the questions for which the objective requires answers. If you cannot do this, then you do not understand the problem. For example, in the population doubling model, the question was: "When (at what time) will the population be twice its current value?"

2. *What quantities are needed to answer the questions?* In compartment models (and almost all others), objective questions are answered with specific numbers or series of numbers. Write down the required quantities and their units.

   In the population doubling problem, it is the "year" when the population has doubled. The size of the population at doubling is of minor concern in this problem (indeed, given the initial condition, it is trivial to compute).

3. *What equations will answer the questions?* Can you write an explicit dynamic equation (e.g., finite difference equation) whose value at some time will constitute an answer? In the population doubling problem, the answer is "no." We did not solve the problem by writing an equation describing the doubling time. We wrote an equation for population growth and *from this* determined doubling time. If the question had been, "What will the population size be in 1999?" then a dynamic equation would answer it.

   If you can, in principle, answer the question directly with a dynamic equation, then this is at least one of the state variables in the model and it becomes a level in a Forrester diagram. (You do not write the equation at this stage, but simply recognize that such an equation, when written, will answer the question.) If a dynamic equation will not immediately answer the question, then (a) you need an auxiliary equation to compute the answer from another variable, and (b) you need another quantity and state variable that will serve as input to the auxiliary equation. An information flow (dotted line) will connect these two objects. Figure 3.8 illustrates the concept in the relation between **Harvest** (g N) and **Profit** ($). The units of the state variable and the auxiliary variable will almost certainly be different, for otherwise a dynamic equation would have answered the question.

4. *What other primary flow quantities are needed?* From the objectives and prior knowledge or data, write down the quantities that will flow into and out of the state variables that contribute to the question. These flows determine the dynamics of the level. The flows will connect to additional levels by material-transfer arrows in the Forrester diagram. For descriptive purposes only, we will call these the *primary* state variables. In the simple population doubling problem, a single state variable suffices, so there are no others. In Fig. 3.8, a single state variable influences the primary quantity needed for the objectives (**Profit**). But the objectives refer to pesticide and fertilization effects, and we know (or presume) from prior information that the harvest dynamics will be influenced by the size of the crop in the field (**Field Crop**), and this will be influenced by insect consumption (**Pests**). Prior knowledge also tells us that fertilizer is applied to the soil and is subsequently removed from a pool of N contained in the soil. Thus, we hypothesize that a sufficient model would be one that contained the state variables (levels) shown in Fig. 3.8 (i.e., **Soil Nutrient Pool**, **Field Crop**, **Pests**, and **Harvest**).

5. *Is an explicit spatial representation required?* Do the objectives refer to or require knowledge of events at different places? If so, then a transport model (Chapter 1) may be appropriate or the primary state variables should be replicated at each discrete spatial location. Typically, the state variables at the different spatial locations will be connected by material transfers (immigration or advection).

6. *What are the controls on the flow rates between the state variables?* The controls become influences or information transfers in Forrester diagrams. For each state variable, list the factors influencing the rates of flow into the level and influencing the rates of flow out of the level. In general, there will be four sources of influences: (1) parameters, (2) auxiliary variables whose inputs are from the primary state variables, (3) driving variables, and (4) inputs (possibly via auxiliary variables) from state variables other than the primary state variables. Type (1) is illustrated in Fig. 3.10 by the influence of parameter "c" on "birth rate." Type (2) is illustrated in Fig. 3.9 by the loop between "K," "Electrical Potential," and flow rate into "K." Type (3) is illustrated in Fig. 3.8 by the influence of "Fertilization" on the flow rate into "Soil Nutrient Pool." Type (4) occurs, for example, when the primary state variables are defined on one level of biological organization (e.g., population), but secondary state variables at another level of organization (e.g., individual body size) are required to implement hypothesized flow rate controls at the population level. For example, populations with large average body size consume resources faster than populations with small body sizes. If type (4) controls are present, then the secondary state variables must be implemented as levels in a parallel model (Fig. 3.9).

7. *Do you know any parameter names?* If the objectives or prior knowledge suggests important parameters, these should be included in the Forrester diagram. Most of these do not become known until explicit equations are suggested for flow rates and auxiliary variables.

3.7 Model Simplification

Thus far, we have emphasized the mechanics of qualitative model formulation. For a number of practical and esthetic reasons, we wish our models and explanations of biological phenomena to be as simple as possible. On the other hand, biological systems are complex, having many processes and variables that interact in complicated, non-linear ways. It is, therefore, natural when creating a model from a general objective statement, such as we used in our example of pesticide effects on farm profit, to create a model that is more complicated than needed or desirable. There is some evidence that models of intermediate complexity are best (Costanza and Sklar 1985). Being able to simplify a model is almost as important as the ability to formulate it in the first place. Think of it as editing the first draft of an essay. Moreover, in Chapter 2 we stressed the importance of evaluating alternative models in parallel. An excellent approach to creating a family of alternative models is to create a gradient from simple to complex. So, the process of model simplification and its converse, model elaboration, are valuable tools for hypothesis testing. Logan (1994) has formalized this philosophy in what he calls the *composite-modeling* approach. In this approach, one designs an initially large model that contains most of the relevant processes and relations. Afterwards, one reduces the large model into progressively simpler, mathematically more tractable versions that, although simple, maintain links and similarities with the more complete model. The end result is a family of models and tools each of which have uses and applications. Because model simplification is central to these ideas, we now present a few principles for simplifying models (see also Shannon 1975).

Eliminate State Variables Every state variable must have a dynamic equation (differential equation or finite difference equation) as well as parameters and initial conditions. There are two ways to reduce model complexity arising from state variables.

1. *Convert a state variable into a constant (e.g., a parameter) or an auxiliary variable.* For example, in Fig. 3.8 we represented Profit as being influenced by harvested crop nitrogen, whose dynamics were determined by the size of the field crop. However, given that alfalfa is harvested by mowing and collecting a fraction of the field crop, a simpler model would be one in which profit is determined from the current field crop and a parameter representing the simple fraction harvested. If we wished to retain the concept that harvesting occurs at fixed time intervals, we could replace the Harvest state variable with an auxiliary variable that is influenced by Season, Field Crop, and a parameter representing the fraction of the field crop harvested. Profit, then, would be determined by season and the harvestable fraction of field crop.

2. *Aggregate state variables.* In Fig. 3.8, we separated soil nitrogen and crop nitrogen to examine the potential interaction between the timing of applications of fertilizer and pesticide. If we would be willing to drop this aspect of the objectives, then we could lump plant and soil nutrients into a single state variable.

Make "Stronger" Assumptions Complexity also enters models in the form of the equations and functional relationships. For example, we compared the models of population growth with and without density effects on reproduction. The former is more complex than the latter. There are several approaches for simplifying functional relationships, and while we will explore the quantitative relationships in more depth in Chapter 4, we can list two possibilities here.

1. *Convert functions of state variables into constants.* Equation 3.2 hypothesizes that effective birth rate decreases with increasing density. If we assume that this function does not exist, then we have simply a constant (r) that describes birth rate (Eq. 3.1).

2. *Convert nonlinear relationships into linear relationships.* Equation 3.2 is a linear relationship between current population density and birth rate. It is not difficult to imagine a more complex relationship that is a curvilinear function. Thus, Eq. 3.2 is already a relatively simple model.

Remove Temporal Complexity Models with temporal variability have a layer of complexity that can be eliminated as follows.

1. *Convert random models into deterministic models.* As discussed briefly in Chapter 1 and in more detail in Chapter 10, random effects on dynamics can be achieved by allowing parameters to vary randomly in time. These types of models have more parameters than their deterministic counterparts and can produce significantly more complicated dynamics that require greater effort to analyze and understand. Removing randomness simplifies the model.

2. *Convert driving variables to constants.* Driving variables or other time-varying perturbations are another means of allowing parameters and processes to vary in time, due to causes not modeled by internal system dynamics. Removing these variables will simplify the model by reducing the number of parameters and amount of data used as well as simplifying dynamics. The simple population models we have discussed so far have no driving variables.

Remove Spatial Complexity As with time, removing spatial complexity is an important simplification tool. The usual method is to convert a model that explicitly models spatial events to one that ignores spatial differences. In Fig. 3.8, we already made this simplification, because we did not attempt to model spatial differences within our alfalfa field. If we had incorporated spatial effects, then (in one possibility) we would have had additional state variables. This would require, essentially, duplicating the four state variables shown for each of the spatial areas we wished to discriminate. For example, we might distinguish the effects of pesticides and fertilizers on the border of the field from those in the interior of the field. If so, then we would need state variables for **Pests_Inside**, **Pests_Border**, **Field_Crop_Inside**, **Field_Crop_Border**, and so on. Adding space to a model usually greatly increases its complexity, so assuming *spatial homogeneity* is a simplifying assumption.

3.8 Other Modeling Problems

In Chapter 1, we introduced four broad classes of models: compartment, transport, particle, and finite state. Forrester diagrams were designed for and are especially useful in describing compartment models. This modeling approach is an extremely powerful and general framework that has many applications in biology, from ecosystems to enzyme kinetics. It is most useful when the system can be decomposed into flows of material or energy among a finite, but possibly large, number of discrete "pools" or compartments. It can also be used when we are interested in quantities that superficially do not "flow," for example, blood or water pressure in animal and plant physiological systems. By linking many compartments together in complicated ways, compartment models can address complex interconnection networks (e.g., foodwebs of many species). Compartment models can also incorporate elaborate control relationships between variables (e.g., the relationship between fertilization schedules and profit). Nevertheless, the remaining three model classes are conceptualizations of systems for which this approach is not optimal or useful.

3.8.1 Transport Models

Of the remaining three classes of models, transport models are closest to compartment models. In transport models, we have a substance [energy (heat) or a quantity of matter] that flows from spatial point to point. A simple example is the flow of a pollutant along a stretch of river after it is emitted from a point source (e.g., a sewage outfall). A central concept shared with compartment models is a quantity that flows, but a major difference is that there is no clear concept of a finite number of compartments in which the substance resides. Instead, there are, in the continuous formulation, infinitely many points along the river at which some quantity of the substance exists. When we model spatial flows across space in this way, we are using an *Eulerian* frame of reference: the origin of the spatial coordinate system is fixed and the substance moves over this coordinate system.

There are many forces that could influence the flow of the pollutant, but the following simplified view uses two that will illustrate the qualitative model formulation. Advection moves the substance with a physical flow of water from point to point (river flow). Diffusion moves a substance in any direction according to the concentration of the substance around each point. Consider an infinitely short segment of the river along its x direction

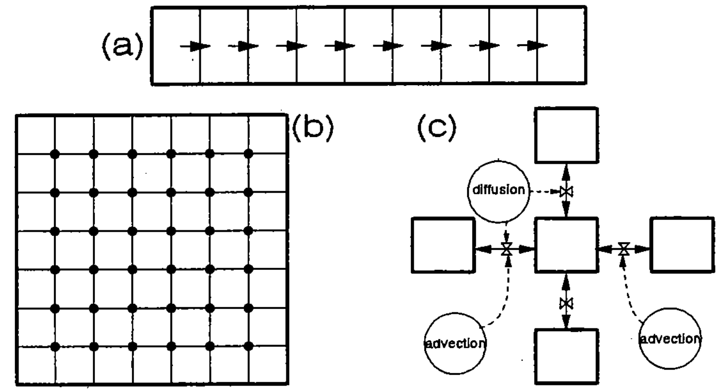

Figure 3.12: (a) Flow between imaginary compartments in a continuous one-dimensional system. (b) Discrete grid system used in two-dimensional transport models. (b) A close-up of five grid points showing the similarity to compartment models.

($\Delta x \to 0$). Figure 3.12a illustrates water and pollutant flows between these infinitely thin segments of river. Since we have rate functions dependent on two variables (space and time), we use partial differential equations based on partial derivatives. For functions of two or more variables [e.g., $f(x,t)$, where x is a spatial dimension and t is time], $\partial f/\partial t$ is the partial derivative of f with respect to t when the spatial variable is held constant. Similarly, $\partial f/\partial x$ is the derivative of f with respect to x when t is fixed. Using this notation, we can write a conceptual rate equation for each segment as:

$$\begin{aligned}\frac{\partial p(x,t)}{\partial t} = & \begin{pmatrix}\text{Advection}\\ \text{In}\end{pmatrix} - \begin{pmatrix}\text{Advection}\\ \text{Out}\end{pmatrix} + \\ & \begin{pmatrix}\text{Diffusion}\\ \text{In}\end{pmatrix} - \begin{pmatrix}\text{Diffusion}\\ \text{Out}\end{pmatrix} + \\ & \begin{pmatrix}\text{Pollutant}\\ \text{Creation}\end{pmatrix} - \begin{pmatrix}\text{Pollutant}\\ \text{Destruction}\end{pmatrix},\end{aligned}$$

where $p(x,t)$ represents the concentration of the pollutant in the water at a point x in space and t in time. Because of the continuous nature of space in this conceptualization, compartment models do not do well here. [There may, of course, be compartments within the river (e.g., fish tissue) wherein the pollutant is stored which we may wish to model and for which compartment submodels will be appropriate.]

However, it happens that many of these models require numerical computations to obtain a solution. This typically requires that we discretize space by imagining it composed of many very closely spaced grid points at which we have obtained a numerical solution and know the pollutant concentration. Figure 3.12b illustrates this for a two-dimensional transport model where we assume the advective flow is unidirectional from left to right and diffusive flow can occur in both directions.

By discretizing space, we have introduced the element that previously distinguished the transport model from the compartment model: a finite number of storage compartments. Figure 3.12c shows a simplified Forrester diagram that illustrates how a compartment model framework could describe the system at one grid point. However, even though we can, after spatial discretization, force the system into the compartment model mode, this does not mean that a Forrester diagram is a felicitous description of the modeled system. It illustrates the forces and processes at a point, but it would be foolish to attempt to represent the spatial scale of Fig. 3.12b with a series of drawings like Fig. 3.12c iterated at each grid point. Since all discrete points are identical, no new information about the structure of the model is revealed by Forrester diagrams at different points.

A second kind of transport model uses a much coarser spatial resolution than that implied by the discretized continuous system above. In ecosystem models, we are often interested in flows of energy or material through a complex foodweb. The foodweb and other processes affecting dynamics, however, are frequently different in space. For example, an ecosystem model of a lake would describe nutrient flow from the physical compartments to plants to herbivores and up through several levels of fish species. Such a model might describe several species at each of these trophic levels, each having complex equations describing nutrient uptake. However, the set of species inhabiting the edges of lakes (littoral zone) differs from those in the open water habitat (pelagic zone), and nutrient inputs from the land obviously will enter the littoral zone. A modeling approach to this framework is to divide the lake ecosystem into two spatial compartments and to divide each of these into the trophic compartments of the biotic part of the system. When such a coarse level of spatial resolution is used, the compartment modeling approach is applicable and a Forrester diagram could be used by separating each biotic compartment in each spatial compartment.

In summary, a compartment model paradigm, in general, and the Forrester diagram approach, in particular, are not always appropriate. This is particularly true when the system is modeled as spatially continuous with small spatial resolution. Nevertheless, at least in early model formulation stages, the compartment model concept can be useful for transport models.

3.8.2 Particle Models

Particle models describe systems in which the variables are physical objects (e.g., billiard balls, or individual organisms) that change in some way according to dynamic equations. This is called the *Lagrangian* frame of reference, as opposed to the *Eulerian* approach of transport models. In general, there can be any finite number of these objects. The objects are characterized as having *essential properties* that are appropriate to the system being modeled and that change according to the dynamic equations.

Most often, especially in physics, the equations define how objects move through space (e.g., planets in a gravitational force field). In this case, the essential properties of objects are their physical position in a coordinate systems [e.g., (x, y, z) in a three-dimensional Cartesian space]. But biological (and physical) models can use a generalization of this framework to include not only spatial position, but other essential properties (e.g., physical properties: mass, momentum, velocity; biological properties: biomass, water content, hunger level). Recently, considerable interest has developed in this class of models in ecology using the name "individual-based modeling" (Huston et al. 1988; DeAngelis and Gross 1992) and human population sciences using the name "micropopulation modeling" (Dyke and MacCluer 1973; Ackerman et al. 1993).

Particle-based models that alter physical position do not fit the compartment model paradigm well, although it is possible. Figure 3.13 shows the physical system and a Forrester diagram for a single prey individual and a single predator individual moving in a 2D space that possesses a refuge for the prey. The state of the prey and predator is defined by their position in space [i.e., their (x, y) coordinates]. It is meaningless to speak of a substance flowing into or out of the "x" or "y" "levels" of the prey or predator, so here the arrow pointing into the position level indicates a small *increase* in the position (e.g., $\Delta x > 0$) and an arrow pointing to the cloud indicates a small *decrease* in the position (e.g., $\Delta x < 0$).

In addition to the artificiality of interpreting position change as a "flow," the compartment model paradigm fails for the same reasons as the discretized transport model. Typically, particle models simulate hundreds or thousands of objects. For complete accuracy, the diagram should be iterated for each of these objects just as it should have been iterated at each spatial point in the discrete transport model. This would add little new information and, in the case of Fig. 3.13, would require a huge number of dotted information transfer lines to indicate the effects of distances between many individuals. So, as with the transport model, Forrester diagrams can be useful for initial model formulation and detailing a subset of the objects and interactions. But it is not useful to describe all of the objects this way.

3.8.3 Finite State Models

Of the four classes of models, finite state models are the furthest from compartment models. As described in Chapter 1, finite state models have no explicit representation of a quantity that flows among pools. In the formulation of the model, we articulate the important states *a priori* and these are the only possibilities allowed. A useful qualitative tool is the state transition graph, which serves a role analogous to that of the Forrester diagram of a compartment model. Each node represents a state and an arrow between nodes represents possible alteration of the system from the state at the end of the arrow to the state at its terminus. Simple finite state models

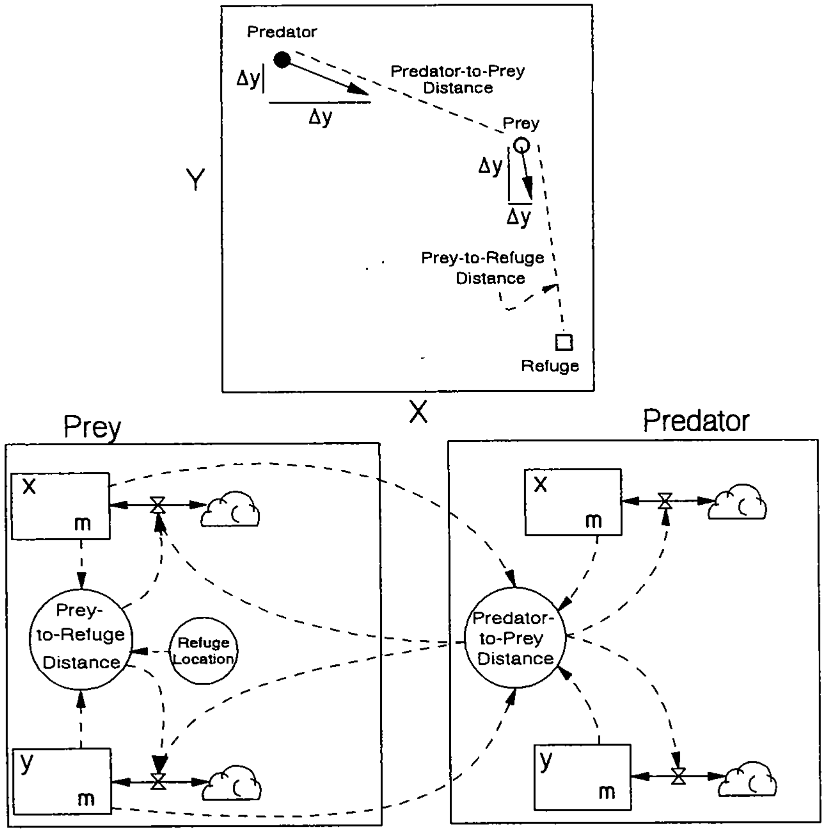

Figure 3.13: Diagram of physical system and Forrester diagram for a particle movement model showing a single predator chasing a prey. The Forrester diagram attempts to represent change in position (Δx, Δy) as a flow to a sink (decrease Δx) or to a level (increase Δx).

(e.g., Markov processes) are stochastic where the arrow is the probability of transition from one state to another; only the current state and the probabilities can affect the outcome. Figure 3.14 shows the transition graph and one stochastic realization for the finite state weather model (Chapter 1). Weather can take one of three states: **G**ood, **I**ntermediate, and **B**ad. A simulation of weather using the transitions probabilities shown on the arrows (Fig. 3.14a) produces a sequence of the three states (Fig. 3.14b). More complex models are possible where, for example, the state of previous time steps can affect the transition probabilities, or other events and conditions in the system can affect the probabilities. These models can be written as finite difference equations with appropriate discretization of the states. Similarly, the model can also be represented as a Forrester diagram (Fig. 3.14c), but it is a clumsy approximation of the transition graph and

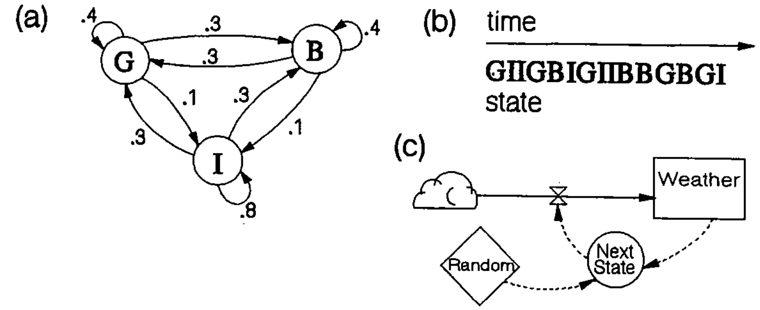

Figure 3.14: A finite state weather model represented as a state transition graph (a), where the numbers represent the probabilities of the transitions denoted by arrows. (b) One stochastic realization of the graph showing the resulting dynamics of states. (c) A Forrester diagram of the model.

the implied flow does not correspond to a physical flow.

3.9 Exercises

1. Assume a substance enters and exits the cell only by passive diffusion. The rate at which passive diffusion transports a substance across a membrane is directly proportional to the difference between the external and internal concentrations. Draw the Forrester diagram for a model in which the ambient concentration is a constant using one state variable, one auxiliary variable, and one rate equation.
2. Consider a substance ("A") that diffuses as above but also is transformed into another substance ("B"). The rate of transformation depends on both the quantities of A and B. Both A and B leave the cell by passive diffusion. Draw a Forrester diagram.
3. Simplify the model represented in Fig. 3.8.
4. Elaborate the model in Fig. 3.8 to include the use of a biological control agent to reduce insect pests on alfalfa. Assume the control agent is a wasp that lays eggs on pest larvae.
5. The classical Lotka–Volterra predator–prey model is:

$$\begin{aligned}\text{Prey:}\quad V_{t+1} &= V_t + rV_t - aV_tP_t \\ \text{Predator:}\quad P_{t+1} &= P_t + abV_tP_t - dP_t\end{aligned}$$

   Assuming the units are a conserved quantity (e.g., g C), draw the Forrester diagram. The parameters are defined as: r = prey per capita rate of increase, a = rate of consumption of prey by predator, b = conversion of prey consumed to new predators, and d = predator death rate.
6. Discuss the relation between Levins' concept of model structure based on generality, precision, and realism and each of the strategies for

model simplification. Which strategies generate which type of model structure?

7. Draw a Forrester diagram of a model that describes the dynamics of the vertical position of an aquatic algae cell based on the following description of flotation in prokaryotic aquatic plankton. Blue-green algae use *gas vacuoles* to manipulate their position in the water column. A single gas vacuole consists of closely packed cylinders each of which is enclosed in a pseudo-membrane of pure protein. The vacuoles are continually produced at a relatively constant rate. The vacuoles collapse when their external pressure exceeds a critical threshold. Their gaseous contents are in equilibrium with the surrounding water. The position of the algal cell is regulated by the number of vacuoles. At high light intensities, cytoplasmic turgor pressure (external to vacuoles) increases beyond the critical threshold for vacuole collapse. This both increases the density of the cell medium and causes the cell to sink. Turgor pressure increases because the light stimulates the uptake of K^+ ions and by-products of photosynthesis (e.g., sugars). At low light levels, the turgor pressure is reduced, the gas vacuoles increase in number, and the cell is more buoyant.
8. Draw a Forrester diagram for the dynamics of blood glucose concentration based on the following simple description of the mammalian blood sugar regulation system. Ingestion of glucose raises stomach levels of glucose, which in turn raises blood glucose levels. This causes the pancreas to secrete insulin, which causes increased transport of glucose into the interior of cells. There it is either used as a source of respiratory energy or is stored. In the liver, glucose is stored as glycogen, which is a form that can be easily released to the bloodstream if blood glucose levels fall below a threshold. The liver acts as buffer to maintain blood glucose levels within acceptable limits between bouts of ingestion.

Chapter 4

Quantitative Model Formulation

4.1 From Qualitative to Quantitative

ONE way to understand a complex, mathematical model is to stare at it until it is obvious. This advice can be less than helpful if you do not know what you are looking for. The approach we follow here exploits the fact that biological models are composed of a relatively few, recurring algebraic constructs. Once these patterns are assimilated, building and reading models becomes a matter of knowing when to use the appropriate component.

We cannot begin, however, until we have a qualitative model for a system that specifies the objects; their basic, qualitative interrelationships; and the underlying hypotheses. The next step is to translate these ideas into mathematical equations. One of the major strengths of Forrester diagrams is the relative ease with which the equations can be generated from the diagram. We can now state a few elements of the method to introduce the material that follows.

The boxes of Forrester diagrams represent the objects of interest: the variables whose dynamic quantities we wish to determine over time. For each of these, we must supply a *state (dynamic) equation* that relates the value of the variable at the next point in the future with the current value and all of the inputs to and outputs from the variable's box. Inputs represent absolute rates of gain, and outputs represent absolute rates of loss. Each of the rates are, in general, calculated by complex, nonlinear equations that combine the flow relations and control relations among system components. The rate equations will therefore involve the *parameters*, *auxiliary equations*, and *driving variables* as specified by the Forrester diagram. Summing all of the rate equations for a given state variable yields the net rate of change for that variable at the current point in time. After incrementing time, this calculation is repeated using the state variable values from the previous iteration until the necessary number of solutions is obtained. In the remainder of this chapter, we will provide some general rules for the